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REPORT AND RECOMMENDATIONS FOR IMPROVING CONSTITUTIVE RELATIONS USED IN COMPUTER CODES

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This Technical Report is the product of a series of meetings held at BDM/Washington by the technical staff and consultants of The BDM Corporation at the request of, and in cooperation with, representatives of DARPA. The motivation for holding these meetings, and associated technical analyses, was DARPA's interest in large-scale computer calculations of the effects of strong shocks in solids.

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(1) As a first step toward cultivating productive exchange and collaboration between concerned groups, two three-day workshops are proposed, which are to be spaced approximately six months apart, the first one taking place in the fall of 1983, where approximately twenty-five prominent mechanics researchers and code developers are brought together to discuss and exchange views on major problems of their immediate concern.

(2) As a second step, a yearly two-week seminar is proposed, to take place in a remote relaxed environment, including about twenty-five carefully selected participants, with a format that would encourage and cultivate continued communication and collaboration between the participants.

(3) Finally, it is recommended that the present team, together with one more team member (to be added) with expertise in numerical methods, make a concerted effort to bring together relevant known results in constitutive descriptions of metals and geo-materials, and then present these in a unified format with discussions of their range of applicability and their limitations, and in this manner identify areas in need of further research. This effort should produce a report which may serve as the focal point for the proposed second workshop and the first two-week seminar.

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This Technical Report is the product of a series of meetings held ~~at BDM/Washington~~ by the technical staff and consultants of The BDM Corporation at the request of, and in cooperation with, representatives of DARPA. The motivation for holding these meetings, and associated technical analyses, was DARPA's interest in large-scale computer calculations of the effects of strong shocks in solids.

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SUMMARY

A team consisting of the present writers was brought together to work with Dr. Thomas C. Bache, Jr. of DARPA, and Dr. Martin Stickley and the scientific staff of The BDM Corporation, in an effort to examine the general area of elasto-plastic and visco-plastic material descriptions and their implementation in large computer codes developed for application to problems of interest to the DoD. The team was asked to make recommendations for improving communication and collaboration between solid mechanics researchers whose primary interest is development and practical use of computer codes, and to suggest effective steps which should be taken in order to enhance current capabilities in computational solid mechanics, particularly for application to defense related problems. In addition, the team was required to clarify a few basic concepts in plasticity theory, such as the normality rule and the convexity of the yield surface in relation to Drucker's stability postulate.

This report briefly addresses these and associated issues. In particular, it makes the following specific recommendations:

(1) As a first step toward cultivating productive exchange and collaboration bewteen concerned groups, two three-day workshops are proposed, which are to be spaced approximately six months apart, the first one taking place in the fall of 1983, where approximately twenty-five prominent mechanics researchers and code developers are brought together to discuss and exchange views on major problems of their immediate concern.

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and then present these in a unified format with discussions of their range of applicability and their limitations, and in this manner identify areas in need of further research. This effort should produce a report which may serve as the focal point for the proposed second workshop and the first two-week seminar.

I. INTRODUCTION

A team consisting of the present writers was brought together in order to examine the general area of elasto-plastic and visco-plastic constitutive material descriptions used in large computer codes developed for solving solid mechanics problems of interest to the DoD. We were given a set of documents and we met as part of a panel with Dr. Thomas C. Bache (DARPA), Dr. Martin Stickley (BDM) and other members of the scientific staff of The BDM Corporation in McLean, Virginia on March 15, 1983. The purpose of the meeting was to briefly discuss these documents and more importantly to initiate discussions on possible ways to improve the constitutive descriptions used in some of the large scale government codes that are , in turn, used to address problems of interest to the DoD.

I.1 Nature of the Problem as Explained to us by Dr. Bache

Some concerns of the DoD regarding large scale numerical calculations in the area of continuum mechanics performed with Lagrangian finite difference codes developed in government laboratories were outlined by Dr. Bache during the panel discussions of March 15, 1983. From this oral briefing and the concomitant discussion it appears that the central issues as perceived by the DoD are as follows:

i) There is currently insufficient communication and collaboration between solid mechanics researchers whose primary interest is inelastic constitutive material characterization, and numerical analysts whose primary interest is the development and practical use of large computer codes for complex defense related problems;

ii) there is a range of methodologies used in large computer codes, some of which are not easily understood or assessed within an established mechanics framework, which, in turn, renders both self evaluation and peer review difficult; and

iii) this deficiency in communication and collaboration between the research and development communities in university, industry, and government is hampering progress toward the development of more reliable methods for solving problems of interest to DoD.

It should be noted that these concerns expressed by Dr. Bache were very specifically directed at codes that are based on Lagrangian finite-difference methods. However, the basic issues seem to involve the vital characteristics of constitutive material description, as well as the translation of the constitutive relations into numerical algorithms. Over the past ten years or so, it has become clear that subtle deviations from classical concepts of elasto-plasticity may have profound effects even on the qualitative characteristics of the solutions of initial boundary-value problems. Some of these issues are at the frontier of our current understanding of the mechanical behavior of solids. Others may have emerged because of the lack of communication between those concerned with material characterization and those concerned with its practical implementation in numerical codes. In the first case, technological and geo-materials of current interest require material descriptions which may not follow the classical concepts such as normality and associative flow rule. Little is known about the character of the solution, its sensitivity to small perturbations in data, its uniqueness, and its other vital attributes, when deviations of this kind are mandated by the physics of the material. In the second case, on the other hand, uncertainties in the quality of the solution may be brought about by the involved numerical schemes which inadvertently may introduce changes into the most fundamental characteristics of the intended constitutive relations. The extent and the practical implications of these problems are not clear to the present team, nor, apparently, to DoD. They must be brought to light and examined by providing a forum for self-evaluation and communication between concerned groups.

I.2 General Comments

There is in general, we believe, a good deal of exchange of information among numerical analysts and solid mechanicians working in some government laboratories and those in industry and university. Furthermore, there currently exists an impressive range of research and development activity in computational mechanics and in constitutive modeling of

inelastic response of materials. This activity takes place in industry, government, and university, and has led to some accurate and reliable methods for solving complex problems in elasto-plasticity. Access to these developments is available in many ways including the open research literature, professional society meetings and special symposia, and commercial numerical codes. The more successful efforts in the field have, we believe, developed around application of the principles of mechanics established for elastic-plastic and visco-plastic continua, which are themselves the subject of continual open and thorough review by the mechanics community and, therefore, they are continually changed and improved.

What would therefore seem to be of value in addressing some of the concerns expressed by Dr. Bache listed above is a means of bringing this existing expertise and knowledge into the clear view of those working on complex defense problems. This would be of value to those wishing to improve their codes or to obtain help, or the means for solving problems or for defining the limitations of these solutions, as well as for deciding what specific new research or development is needed. For these purposes our main recommendation, outlined in Section II, is that DARPA as a first step sponsor a series of workshops the purpose of which is to foster communication, cooperation, and collaboration among those individuals involved with solving complex defense related problems and others in the mechanics community at large.

I.3 Nature of Immediate Task as Discussed with Dr. Bache

From the examination of the documents provided us, and discussion with Dr. Bache it appears that our immediate task consists of the following:

i) To make recommendations and to work with DARPA in trying to foster helpful communication and collaboration between the concerned groups;

ii) to make recommendations for further research which will enhance constitutive material descriptions and their implementation in large defense related computer codes; and

iii) to clarify those concepts in plasticity theory which are germane to the panel's discussions. The brief discussion we give in Appendix A is aimed at the panel itself.

I.4 Organization of This Report

This report is organized around the three items mentioned above in Section I.3 In Section II we submit a set of recommendations which we believe will foster communication and, we hope, collaboration between the mechanics community and numerical analysts working on large complex numerical problems of interest to the U.S. Government. In Section III we outline the team's possible tasks which may continue after the present reporting period.

In Appendix A we briefly discuss some key concepts in plasticity theory which have emerged during the course of our discussion with Dr. Bache and scientific staff members at The BDM Corporation, an understanding of which by all parties participating in the panel discussions will be useful for proceeding with the remaining two tasks outlined above. In particular, Drucker's stability postulate is discussed in a very simple manner in relation to the concepts of normality, convexity, and constitutive inequalities in rate independent plasticity.

II. RECOMMENDATIONS FOR FOSTERING COMMUNICATION AND COLLABORATION BETWEEN CONCERNED GROUPS

Over the past two decades, considerable progress has been made in experimental and theoretical characterization, as well as in numerical modeling of thermomechanical behavior of technological and geo-materials. A great deal has been learned about the constitutive description of material response under various loading conditions. The limitations and the range of applicability of various constitutive assumptions have become clearer and various numerical schemes appropriate to a wide class of problems have been developed. While much remains to be explored in all these areas, all in all, a great deal of information and methodology

already exists within the field of solid mechanics which should be utilized in modern numerical codes.

Therefore, a major task ahead appears to be the creation of an environment which is naturally conducive to the free exchange of information and which would provide a forum for self-evaluation, as well as mutual appreciation of needs and limitations of numerical methods and material models. We must seek to provide a natural basis for productive collaboration between concerned groups.

As a first step toward this, we propose two three-day workshops spaced approximately six months apart, the first one taking place early in the fall of 1983, where approximately twenty-five prominent mechanics researchers and code developers are brought together to discuss and exchange views on major issues of their immediate concern. The cost of the participation of these invitees will be borne by DoD. However, the meeting would be open to others, who may attend at their own cost, and who would participate in the discussions. The format of the meeting, as well as the composition of the invited participants will be worked out in consultation with Dr. Bache and other appropriate DoD personnel, in an effort to optimize the effectiveness of the workshop. There should be a few somewhat tutorial lectures, along with lectures on current research, followed by ample discussions.

As a second step toward cultivating communication and collaboration between the various groups, we propose that a yearly two-week seminar be established to take place in a relaxed, possibly remote, quiet setting, where approximately twenty-five key individuals from academic, industry, and government laboratories are brought together in order to discuss and actually work out technical problems essential for effective simulation of structural and material response. The composition of this group should be carefully defined, in order to bring about effective exchange and, we hope, extensive and continual collaboration. In this regard, it may be important to ensure a certain continuity, while at the same time allow for fresh ideas and renewed participation.

Summary of Recommendations

(1) A three-day workshop to be held in the early fall of 1983, consisting of about 25 invited participants, with expenses covered, and other interested participants who may attend at their own expense. The format of the meeting and the composition of the participants should be worked out, in order to optimize technical exchange.

(2) A similar workshop as (1) above, to follow approximately six months later, early spring of 1984.

(3) A yearly two-week seminar in a remote relaxed environment, including about 25 carefully selected participants, with a format that would encourage and cultivate continued communication and collaboration between the participants.

III. RECOMMENDATION FOR FURTHER TECHNICAL EFFORT IN CONSTITUTIVE MATERIAL DESCRIPTION

As pointed out in Section II, already a great deal has been learned about various constitutive material descriptions and their effectiveness as well as their limitations, which should be incorporated in any advanced computer code. The greatest part of this work has been sponsored by governmental agencies such as NSF, NASA, DOE, and various scientific offices of DoD. Furthermore, it is expected that these agencies will continue to support fundamental research and development, both experimental and theoretical, in the area of materials characterization. Nevertheless, there are a number of important areas in material characterization as well as its accurate implementation in computer codes, which would benefit by additional funding.

To identify these research areas, a careful evaluation of existing capability, at least as far as it relates to the computer codes of interest to DoD should be made. In the course of this evaluation, areas of immediate research needs should be identified, which may then receive specific funding or may be given prominence and special attention by appropriate DoD research sponsoring offices.

In order to accomplish these objectives in an efficient and meaningful way, we recommend that the tasks of the present team be continued beyond the termination of the present reporting schedule, until shortly after the completion of the second three-day workshop recommended in Section II above. We recommend that the team's tasks should include the following:

(1) To serve as the scientific committee for the workshops recommended in Section II, to prepare, in consultation with appropriate DoD personnel, the format of the meetings and composition of the invited participants, and to serve as coordinators of the meetings.

(2) Together with one more team member (to be added) with expertise in numerical methods, to make a concerted effort to bring together relevant known results in constitutive material description for elasto-plastic and visco-plastic solids at various pressures and temperatures, for application to metals as well as to geo-materials, and to present these in a coordinated and unified format, together with careful discussions of their range of applicability, their limitations, and hence in this manner identify areas in need of further research. The details and the timetable for this and related matters are to be worked out in consultation with appropriate DoD personnel. This effort should produce a rather comprehensive report which may serve as the focal point for the proposed workshops and the first two-week seminar, recommended under Section II above.

(3) To assist the appropriate DoD personnel with the evaluation of unsolicited proposals in areas of constitutive material description and its numerical implementation, as well as to formulate statements for soliciting research proposals in these areas.

APPENDIX A. CERTAIN CONCEPTS IN PLASTICITY

A.1 Drucker's Postulate

a) Background: By the early 1940's linear elasticity was a well-developed complete theory, where field equations and constitutive relations were fully understood, and where existence and uniqueness theorems, as well as fundamental minimum principles, provided guidance for analytical and numerical solutions of various (elasticity) problems. However, the same was not the case for plasticity.

Drucker's stability postulate was an attempt to provide similar guidance for the solution of plasticity problems; see, e.g., Drucker (1950), and Martin (1975). This postulate is not (as clearly stated by Drucker and others) a thermodynamic requirement. It is a restriction on constitutive relations, and is used to classify materials. It does not necessarily apply to all materials whose response may be classified as "plastic." However, once accepted for a particular class of materials (usually at small strains), it immediately leads to normality of the plastic strain rate on the yield surface at smooth points, to convexity of the yield surface, and confines the direction of plastic strain rates within the outward normals at vertices and corners of the yield surface. Drucker's postulate precludes nonconvex yield surfaces when the elastic properties remain the same in the course of plastic flow (which is essentially the case for most metals up to moderate strains). When the elastic properties change because of plastic flow (which is often the case for most geo-materials and also concrete), Drucker's postulate does not necessarily imply convexity, but does yield normality. When strains and rotations are large, the Drucker postulate is not free from ambiguity inasmuch as it can be stated in terms of objective rates of different stress measures conjugate to different strain measures. We will not discuss this issue here but only note, as a starting point for further study, the well known papers by Hill (1968) where some implications of the choice of strain measure for the Drucker inequality and other constitutive inequalities are discussed.

b) <u>What is Drucker's Postulate?</u>: Drucker considers a stressed elastoplastically deformed solid (or structure), and postulates that the net work done by an external agency in applying and removing an incremental set of loads or stresses to this solid should be non-negative. The postulate takes the form of an inequality stating that the product of stress rate and strain rate is non-negative. Before we examine the implications of this postulate in elasto-plastic deformation we review some basic concepts in plasticity.

c) <u>Yield Function</u>: The yield function in stress-space idealizes the locus of points within which the state of the material is regarded to be elastic, and on which the state is elasto-plastic. At a given material state, a stress-state outside the yield surface is not admitted. This is a generalization of the uniaxial stress-strain curve for most metals; see Fig. 1a,b. When the yield function is independent of pressure, the material is plastically pressure-insensitive. This is true for many metals at even rather large pressures. However, it is certainly not so for geomaterials, nor for certain pressure-sensitive metals whose yield stress changes with the confining pressure (e.g. some high-strength steels), although in this latter case, the pressure-dependency is not very substantial at moderate pressures.

d) <u>Work-hardening</u>: When the yield surface remains unchanged as plastic flow proceeds, the material is called elastic-perfectly-plastic. If the yield surface expands isotropically as the plastic flow proceeds, then the material is called isotropically hardening. If the yield surface does not change in shape but moves in the stress space, as the plastic deformation proceeds, we have kinematic hardening. Many polycrystalline solids are such that their description appears to require combined isotropic-kinematic hardening. Furthermore, since the plasticity of common crystalline solids essentially stems from slip on crystallographic planes in single crystal constituents,* the yield surface for the polycrystal

* Again for simplicity we will not attempt to discuss inelasticity arising from diffusion at high temperatures, twinning or grain boundary sliding. The important case of inelastic deformation by slip is the only mechanism referred to here.

(and, of course, for the single crystal) invariably forms, upon continued plastic flow, a vertex or a corner. Micromechanical modeling suggests that such vertices are not concave, but rather existing models and experimental results point to convex vertices.

The material is called work-softening if the yield surface shrinks as plastic flow proceeds.

e) Mathematical Statement of Drucker's Postualate; Normality and Convexity: Let $\underset{\sim}{\sigma}$ be the stress tensor, $\underset{\sim}{\varepsilon}$ the strain tensor, and denote their rectangular Cartesian components, respectively, by σ_{ij} and ε_{ij}, $i,j = 1,2,3$. The yield surface is defined by $f(\underset{\sim}{\sigma},\underset{\sim}{H}) = 0$, where $\underset{\sim}{H}$ stands for a set of scalar parameters which characterize the microstructural changes that accompany plastic flow and, for example, lead to material hardening.

Points inside the yield surface define elastic states. For continued plastic flow, stress state remains in the yield surface which changes in view of the associated microstructural variations. Hence, we have, after an increment of loading, $d\underset{\sim}{\sigma}$, a new yield surface defined by $f(\underset{\sim}{\sigma} + d\underset{\sim}{\sigma}, \; \underset{\sim}{H}+d\underset{\sim}{H}) = 0$; Fig. 2.

For continued plastic flow,

$$f = 0, \quad df \equiv \frac{\partial f}{\partial \sigma_{ij}} d\sigma_{ij} + \frac{\partial f}{\partial \underset{\sim}{H}} \cdot d\underset{\sim}{H} = 0, \tag{1}$$

where repeated indices are summed. The plastic loading is defined by

$$\frac{\partial f}{\partial \sigma_{ij}} d\sigma_{ij} \geq 0, \tag{2}$$

with the equality sign corresponding to the neutral loading. For the elastic unloading, on the other hand, we have

$$\frac{\partial f}{\partial \sigma_{ij}} d\sigma_{ij} < 0. \tag{3}$$

Consider an admissible stress-state, $\underset{\sim}{\sigma}^a$, and a cycle of loading to $\underset{\sim}{\sigma}^b$ and unloading back to $\underset{\sim}{\sigma}^a$. The net work over this <u>stress</u> cycle, according to Drucker's postulate, must be non-negative,

$$\oint(\sigma_{ij}^b - \sigma_{ij}^a)d\varepsilon_{ij} \geq 0. \tag{4}$$

Let this stress cycle involve an increment of plastic strain, $d\underset{\sim}{\varepsilon}^p$, and assume that the elastic properties remain unchanged. Then (4) yields

$$(\sigma_{ij}^Y - \sigma_{ij}^a)d\varepsilon_{ij}^p \geq 0 \tag{5}$$

which must hold for any state $\underset{\sim}{\sigma}^a$ in or on the yield surface, and any $\underset{\sim}{\sigma}^Y$ <u>on</u> the yield surface. Hence $d\underset{\sim}{\varepsilon}^p$ must be normal to the yield surface at smooth points, and, at corners, it must be within the outward normals to the surface; see Fig. 3a,b. Moreover, (5) excludes concavity at any point on the yield surface.

<u>We thus have</u>

$$\dot{\underset{\sim}{\varepsilon}}^p = \lambda \frac{\partial f}{\partial \underset{\sim}{\sigma}} \tag{6}$$

<u>from Drucker's postulate, with</u> f = 0 <u>a convex surface</u>.

The total strain rate, $\dot{\underset{\sim}{\varepsilon}}$, is

$$\dot{\underset{\sim}{\varepsilon}} = \dot{\underset{\sim}{\varepsilon}}^e + \dot{\underset{\sim}{\varepsilon}}^p, \tag{7}$$

where (for small deformations)

$$\dot{\varepsilon}_{ij}^e = M_{ijk\ell}\,\dot{\sigma}_{k\ell}, \qquad i,j,k,\ell = 1,2,3; \tag{8}$$

here $\underset{\sim}{M}$ is the elastic compliance. From (6), (7), and (8) we have

$$\dot{\varepsilon}_{ij} = M_{ijk\ell}\,\dot{\sigma}_{k\ell} + \lambda \frac{\partial f}{\partial \sigma_{ij}}, \tag{9}$$

where $\lambda = 0$ for elastic loading and unloading.

It can be shown (Martin (1975)) that the normality rule and the convexity of the yield surface lead to the uniqueness of (well posed) incremental boundary-value problems when the material work-hardens. For an elastic-perfectly-plastic material, the stress increment is unique but not necessarily the strain increment.

Note that when the material is plastically incompressible, then only the deviatoric stress enters the definition of the yield surface. In this case, $\dot{\varepsilon}^p_{kk} = 0$.

When f depends on only the basic invariants of $\underset{\sim}{\sigma}$, then the plastic strain-rate tensor is coaxial with the stress tensor (they have the same principal directions). This is called "coaxiality." Micromechanical changes induced by plastic flow often lead to non-coaxiality. The notion of kinematic hardening has been introduced in order to account for this. In this case the yield function is written in terms of $(\underset{\sim}{\sigma} - \underset{\sim}{\beta})$, where $\underset{\sim}{\beta}$ defines the center of the yield surface. An evolutionary equation is needed to define $\underset{\sim}{\beta}$, e.g., $\dot{\underset{\sim}{\beta}} = A\dot{\underset{\sim}{\varepsilon}}^p$; see, e.g., Mróz et al. (1976).

f) Comments on Physical Basis of Normality: A simple model for elastic-plastic deformation of single crystals results if we assume that plasticity stems from slip over active crystallographic slip planes, and the elasticity from lattice distortion which produces a compatible overall deformation. Let there be N active slip systems. The α^{th} slip system is defined by the unit normal $\underset{\sim}{n}^\alpha$ of the slip plane, and the unit vector $\underset{\sim}{s}^\alpha$ in the direction of slip. The plastic strain rate then is (Bishop and Hill (1951), Taylor and Elam (1926), and others*)

$$\dot{\varepsilon}^p_{ij} = \sum_{\alpha=1}^{N} \tfrac{1}{2}(n_i^\alpha s_j^\alpha + n_j^\alpha s_i^\alpha)\dot{\gamma}^\alpha, \tag{10}$$

* See, e.g., Asaro (1979, 1983), Havner and Shalaby (1977), Nemat-Nasser (1983), Nemat-Nasser et al., (1980), and Rice (1971, 1975) for rather comprehensive accounts.

where $\dot{\gamma}^{\alpha}$ is the slip rate. Note from (10) that $\dot{\varepsilon}^{p}_{ii} = 0$. According to this model, the slip induced plastic flow is incompressible.

The resolved shear stress, τ^{α}, acting in the slip direction is

$$\tau^{\alpha} = \sigma_{ij} n_i^{\alpha} s_j^{\alpha} = \sigma_{ij}\, \tfrac{1}{2}(n_i^{\alpha} s_j^{\alpha} + n_j^{\alpha} s_i^{\alpha}) \qquad (\alpha \text{ not summed}).$$

According to Schmid's law, for an active slip $\tau^{\alpha} = \tau_Y^{\alpha}$, where τ_Y^{α} is the current local yield stress in shear. The slip is inactive if $\tau^{\alpha} < \tau_Y^{\alpha}$. The rate of plastic dissipation is

$$\sigma_{ij}\dot{\varepsilon}^{p}_{ij} = \sigma_{ij} \sum_{\alpha=1}^{N} \tfrac{1}{2}(n_i^{\alpha} s_j^{\alpha} + n_j^{\alpha} s_i^{\alpha})\dot{\gamma}^{\alpha} = \sum_{\alpha=1}^{N} \tau^{\alpha}\dot{\gamma}^{\alpha} = \sum_{\alpha=1}^{N} \tau_Y^{\alpha}\, \dot{\gamma}^{\alpha}. \tag{11}$$

Now, consider a stress state σ^{*}_{ij} inside the current yield surface. The corresponding resolved shear stress, $\tau^{\alpha *}$, for the α^{th} slip system then satisfies $\tau^{\alpha *} \leq \tau_Y^{\alpha}$. Thus

$$(\sigma_{ij} - \sigma^{*}_{ij})\dot{\varepsilon}^{p}_{ij} = \sum_{\alpha=1}^{N} (\tau_Y^{\alpha} - \tau_Y^{\alpha *})\dot{\gamma}^{\alpha} \geq 0 \tag{12}$$

which reduces to (5) if we note that σ_{ij} is on the yield surface $(\sigma_{ij} = \sigma^{Y}_{ij})$ and σ^{*}_{ij} is inside or on the yield surface $(\sigma^{*}_{ij} \equiv \sigma^{a}_{ij})$.

The above model may be modified to include non-Schmid effects, plastic volumetric strain, and friction. This will immediately show that the plastic strain rate can no longer be normal to the yield surface (which, for frictional materials, will depend on pressure). In this case, one may still have a "plastic potential," g, such that

$$\dot{\underset{\sim}{\varepsilon}}^{p} = \lambda \frac{\partial g}{\partial \underset{\sim}{\sigma}}\,, \tag{13}$$

but this plastic potential, in general, will not coincide with the yield surface; for discussions, examples, and references, see Asaro and Rice (1977) and Nemat-Nasser _et al_. (1980, 1983).

g) _Comments on Thermodynamic Basis of Normality_. Since the inelastic response of solids stems from micro-structural changes, one reasonable way to account for this is to introduce a set of _internal_ state

variables, collectively denoted by $\underset{\sim}{\xi}$, in such a manner that the response is <u>elastic</u> when $\underset{\sim}{\xi}$'s remain unchanged, i.e., when no micro-structural changes occur. While this may not be the most general approach, it serves to illustrate the kind of assumptions which are required in order to yield flow potentials for inelastic strain rates. (These assumptions are in addition to the basic requirement of non-negative dissipation.) For simplicity, we assume that $\underset{\sim}{\xi}$'s are n independent scalar parameters, ξ_α, $\alpha = 1,2,\ldots,n$.

Since for $\underset{\sim}{\xi}$= constant the response is elastic, the Helmholtz free energy $\phi = \phi(\underset{\sim}{\varepsilon},\theta;\underset{\sim}{\xi})$ and the Gibbs function $\psi = \psi(\underset{\sim}{\sigma},\theta;\underset{\sim}{\xi})$ exist with the following properties*:

$$\underset{\sim}{\sigma} = \frac{\partial\phi}{\partial\underset{\sim}{\varepsilon}}, \qquad \eta = -\frac{\partial\phi}{\partial\theta}, \qquad \underset{\sim}{\Lambda} = -\frac{\partial\phi}{\partial\underset{\sim}{\xi}}, \tag{14}$$

$$\underset{\sim}{\varepsilon} = \frac{\partial\psi}{\partial\underset{\sim}{\sigma}}, \qquad \eta = \frac{\partial\psi}{\partial\theta}, \qquad \underset{\sim}{\Lambda} = \frac{\partial\psi}{\partial\underset{\sim}{\xi}}, \tag{15}$$

where θ and η are the temperature and entropy-density, respectively; $\underset{\sim}{\Lambda}$'s are the thermodynamic <u>forces</u> conjugate to $\underset{\sim}{\xi}$'s; and ϕ and ψ are related by a Legendre transformation as follows:

$$\phi + \psi = \sigma_{ij}\varepsilon_{ij}. \tag{16}$$

By definition, the inelastic strain-rate is caused by the changes in internal variables, $\underset{\sim}{\xi}$'s, only. Hence, we have

$$\dot{\underset{\sim}{\varepsilon}}^{p} = \frac{\partial\underset{\sim}{\varepsilon}}{\partial\xi_\alpha}\,\dot{\xi}_\alpha, \qquad \alpha = 1,2,\ldots,n \qquad\qquad (\alpha \text{ summed}), \tag{17}$$

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* The differentiation denoted by the operator "$\partial/\partial\ldots$" implies derivative with respect to the indicated variable with <u>all</u> other variables held fixed.

and, in view of (15),

$$\dot{\underset{\sim}{\varepsilon}}^{P} = \frac{\partial^2 \psi}{\partial \xi_\alpha \partial \underset{\sim}{\sigma}} \dot{\xi}_\alpha = \frac{\partial \Lambda_\alpha}{\partial \underset{\sim}{\sigma}} \dot{\xi}_\alpha \qquad (\alpha \text{ summed}). \tag{18}$$

The evolution of the internal variables must be prescribed on the basis of the involved physical processes. This must be guided by experimental observations. The only basic requirement is that the dissipation rate be non-negative, i.e.

$$\Lambda_\alpha \dot{\xi}_\alpha \geq 0 \qquad (\alpha \text{ summed}). \tag{19}$$

Depending on the type of evolutionary equations used, the inelastic strain-rate, $\dot{\underset{\sim}{\varepsilon}}^{P}$, may or may not admit a potential.

In some applications it may be reasonable to regard each flux, $\dot{\xi}_\alpha$, dependent explicitly on only its own conjugate force Λ_α, as well as (in general) on the temperature θ, but not on other forces nor explicitly on the overall strain, $\underset{\sim}{\varepsilon}$; note, however, the implicit dependence on $\underset{\sim}{\varepsilon}$ through Λ_α. The Schmid law of Subsection f) above is of this kind. Other physical examples are discussed by Rice (1971, 1975). In cases of this kind, or even in more general settings, one may express $\dot{\underset{\sim}{\xi}}$'s as

$$\dot{\underset{\sim}{\xi}} = \lambda \frac{\partial \Omega}{\partial \underset{\sim}{\Lambda}}, \tag{20}$$

where $\Omega = \Omega(\underset{\sim}{\Lambda}, \theta)$. From (20) and (18) it then follows that

$$\dot{\underset{\sim}{\varepsilon}}^{P} = \lambda \frac{\partial \Omega}{\partial \Lambda_\alpha} \frac{\partial \Lambda_\alpha}{\partial \underset{\sim}{\sigma}} = \lambda \frac{\partial g}{\partial \underset{\sim}{\sigma}}, \tag{21}$$

$$g(\underset{\sim}{\sigma}, \theta; \underset{\sim}{\xi}) \equiv \Omega(\underset{\sim}{\Lambda}(\underset{\sim}{\sigma}, \theta; \underset{\sim}{\xi}), \theta). \tag{22}$$

Note that (20), and hence (21), is always valid if the fluxes, $\dot{\underset{\sim}{\xi}}$, are related linearly to the forces, $\underset{\sim}{\Lambda}$, and the Onsager reciprocal relations hold (the classical irreversible thermodynamics). In this case, the flow potential g is proportional to the (isothermal) rate of entropy production

associated with the plastic flow. In general, however, (20), and hence (21), is an additional constitutive assumption, beyond any basic thermodynamic requirements. The normality rule (21) does not stem from the second law of thermodynamics.

A.2 Implications of Constitutive Assumptions

The inter-related concepts of normality, convexity, and constitutive structure outlined above have also served as the starting points for discussions of stability and of uniqueness of solutions to boundary value problems, at small strains (e.g., see Drucker (1950) or Martin (1975)). It is not surprising then that deviations from normality, for example, or even subtle changes in yield surface shape (when convexity is maintained), have vital influence on the most important qualitative features of the plastic deformation process. For example, in the last 10 years or so there has been a great deal of interest in obtaining more precise predictions and descriptions of nonuniform and localized modes of plastic deformation*. Much of this research has been aimed at describing the localization of plastic flow as a "constitutive instability" rather than the result of, for example, microfractures in progress or severe "geometrical" or "material" imperfections. Most of this work accounts for the important effects of large strains (and rotations) and has shown that both deviations from normality and the existence of corners on (convex) yield surfaces can lead to intensely localized straining in homogeneous, strain hardening materials where otherwise (i.e. with normality and smoothness of the yield surface) strain softening behavior would have been required.

As a specific case, consider uniaxial extension of a uniform metallic bar. It is a well-known experimental fact that at a certain stage of axial tension, the specimen begins to neck, and then, very often, localized shear bands develop within the necked region. If Mises' yield function

* See, e.g., Asaro (1979), Hill and Hutchinson (1975), Iwakuma and Nemat-Nasser (1983), Needleman and Rice (1978), Nemat-Nasser et al. (1980), and Rice (1976).

together with positive work hardening is used, it is well known that no such localized shear deformation can be predicted analytically for any finite strain. On the other hand, if one appropriately modifies the flow rule in such a manner that the plastic strain increment also has a component tangent to the yield surface, then the theory will predict, with suitable adjustment of the parameters, localized shear bands in the necked region at reasonable finite strains; see Hill and Hutchinson (1975), Iwakuma and Nemat-Nasser (1982), Rice (1976), and Storen and Rice (1975). It is, therefore, seen that a computer code with an algorithm which advertently or inadvertently introduces a tangential component for the plastic strain increment is, in fact, introducing a major alteration into the constitutive description which, with appropriate mesh structure, could actually predict instabilities that may be outside the realm of the prediction of the considered yield condition. Such a numerically induced change in the most essential character of the constitutive relations is clearly undesirable, since, inter alia, it may render the results nonunique and calculation-dependent.

These comments serve to underscore the vital need for careful materials characterization in constitutive descriptions as well as an equally careful translation of constitutive relations into numerical algorithms. These considerations should be incorporated in future panel discussions and most importantly in the lectures and discussions associated with the workshops we proposed in Section II.

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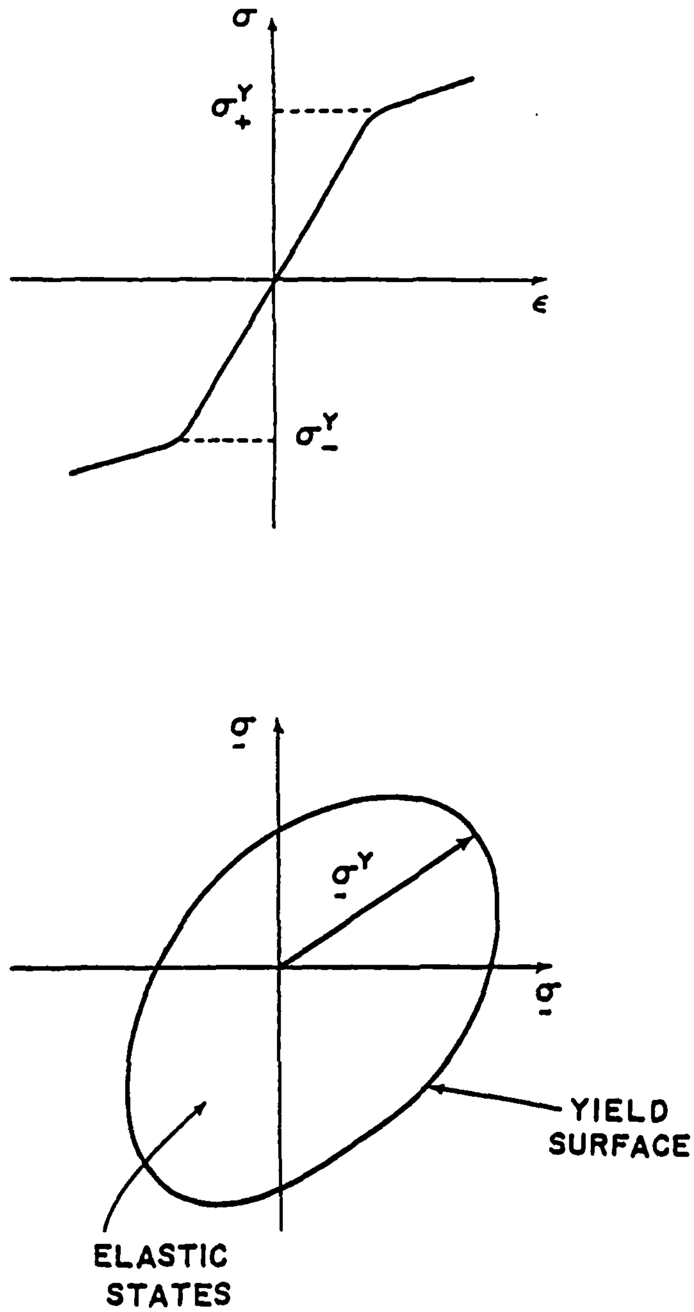

Figure 1. (a) The uniaxial stress-strain curve; σ_+^Y and σ_-^Y are the initial yield stresses in tension and compression, respectively.

(b) The yield surface in the stress-space; points inside this surface represent elastic states.

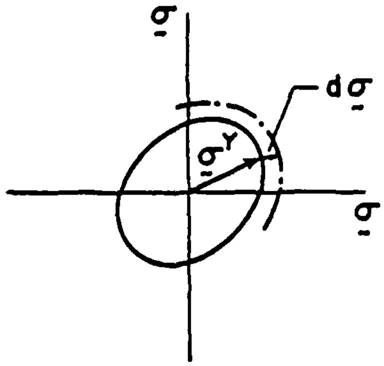

Figure 2. Change in the yield surface caused by an increment in stress, $d\underset{\sim}{\sigma}$

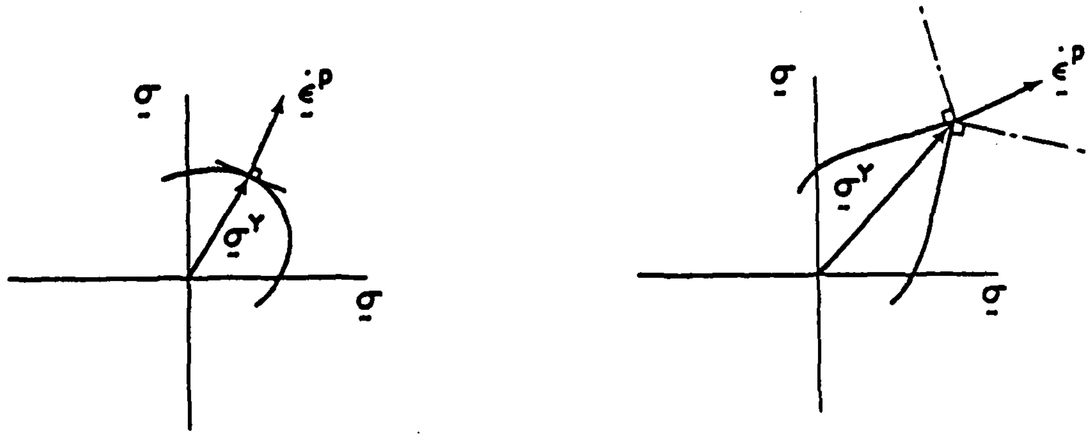

Figure 3. (a) Normality rule, and the convexity of a smooth yield surface.

(b) Convexity at a vertex.